

Resonant Soft x-ray emission investigation of Be-chalcogenide thin films and superlattices

D. Eich¹, U. Groh¹, R. Fink¹, C. Heske^{1,2}, M. Keim¹, G. Reuscher¹, A. Waag¹, A. Fleszar³, M.M. Grush⁴, T.A. Callcott⁴, D.L. Ederer⁵, R.C.C. Perera⁶, and E. Umbach¹

¹ Experimentelle Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

² Advanced Light Source, Ernest Orlando Lawrence Berkeley National Laboratory,
University of California, Berkeley, California 94720, USA

³ Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

⁴ University of Tennessee, Knoxville, Tennessee 37996

⁵ Tulane University, New Orleans, LA 70118, USA

⁶ Ernest Orlando Lawrence Berkeley National Laboratory, University of California, Berkeley, California 94720, USA

INTRODUCTION

Since the first demonstration of blue-green laser diodes on the basis of ZnSe [1], II-VI heterostructures have attracted considerable interest in view of potential applications in optoelectronics. Recently, the new class of Be-chalcogenides with novel and interesting properties have obtained remarkable attention. Significant improvements are expected from the use of Be-based heterostructures, since these materials are harder as compared to conventional II-VI materials. Thus the dislocation density is much lower than for, e.g., ZnSe/ZnTe heterostructures, which in turn improves the lifetime of the devices drastically.

Despite the technological relevance of BeTe very little is known about its band structure, as well as about the stability, abruptness, and atomic intermixing of the BeTe/ZnSe interface. Using molecular beam epitaxy or atomic layer epitaxy techniques the termination of the heterointerfaces can be tailored appropriately, i.e., it is possible to prepare both Zn-Te or Be-Se bonds at the interface. Recent photoemission (PES) investigations [2] of thin BeTe overlayers on ZnSe indicate intermixing over several layers for a BeSe interface and a sharp heterointerface for the ZnTe interface.

The inherent disadvantage of PES is the low probing depth which is limited to a few atomic layers. Therefore the influence of intermixing and interdiffusion in a real heterostructured laser device cannot be determined. Soft x-ray emission spectroscopy (XES), in contrast, offers several advantages for probing buried interfaces of real device heterostructures, for instance bulk sensitivity, elemental and chemical sensitivity and non-destructive depth analysis.

RESULTS AND DISCUSSION

We present results of our ongoing studies (BL 8.0, SXF endstation) of excitation-energy dependent resonant XES measurements of thick BeTe(100) and BeSe(100) layers as well as heterostructure superlattices with different period lengths and interface terminations. The transition from the valence band to the Be 1s core level probes the local partial density of states of the valence band at the Be site. By probing the spectral variations with various excitation energies, band structure information can be extracted, in particular at high symmetry points of the Brillouin zone (BZ). Fig. 1 shows excitation-energy dependent XE-spectra of BeTe(100). To obtain the coherent fraction of each spectrum a high energy spectrum was subtracted from the closer-to-threshold excited spectra with the restriction that the remaining intensities must be positive [3]. The two first coherent spectra of BeTe for $h\nu = 113.5$ eV and $h\nu = 113.7$ eV show maxima at about 3.5 eV and 6 eV below the valence band maximum (VBM). These peak intensities correspond to transitions at the X-point, which is the only k-value with unoccupied states which can be reached with the lowest excitation energy. This can be seen in the band structure plot in Fig. 2, which shows a first-principles calculation of the BeTe band structure obtained within the framework of the density-functional formalism in the local density

approximation [4]. The spectrum for $h\nu = 115.5$ eV shows the highest observed emission energy, which can be associated with transitions at the Γ -point of the BZ: at this k-value of the BZ the conduction bands are flat, which corresponds to a high density of states. Thus the emission observed in this spectrum is dominated by transitions at the Γ -point. The spectra between these two high symmetry points represent an intermixing of different k-values, and a detailed analysis for an exact determination of the corresponding k-values is still in progress.

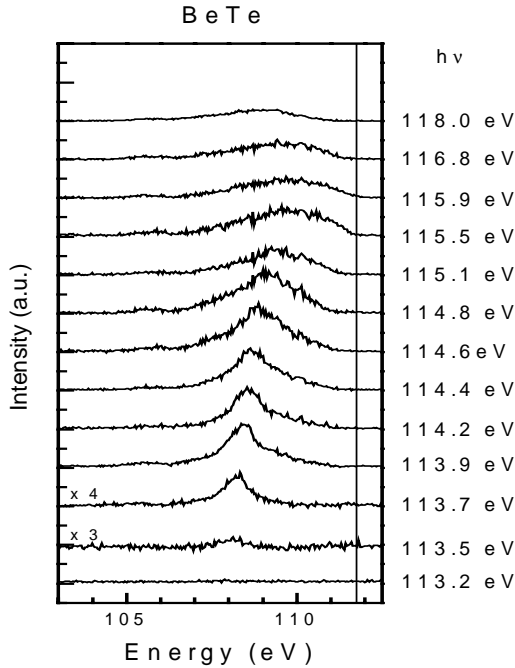


Fig. 1 Excitation-energy dependent XE-spectra of BeTe(100). The spectrum for $h\nu = 113.7$ eV corresponds to transitions at the X-point. The spectrum for $h\nu = 115.5$ eV corresponds predominantly to the Γ -point (highest emission energy).

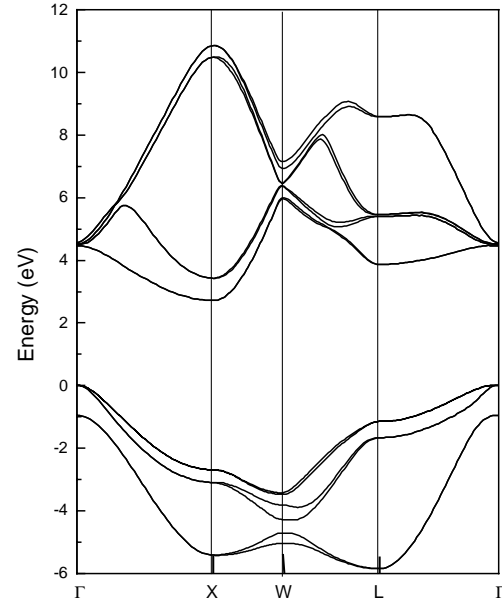


Fig. 2 First-principles calculation of the BeTe(100) band structure obtained within the framework of the density-functional formalism in the local density approximation.

Fig. 3 shows the corresponding valence band XE-spectra of BeSe(100). The excitation energy dependence is weaker for BeSe than for BeTe as is confirmed by band structure calculations, which also show a smaller dispersion of the valence bands. Again the first spectra ($h\nu = 114.1$ eV) correspond to transitions at the X-point, and the spectrum for $h\nu = 116.2$ eV predominantly to transitions at the Γ -point of the BZ. These two sets of excitation-energy dependent valence band spectra of BeTe and BeSe serve as reference spectra for comparison with heterostructure superlattices (SL). We have investigated BeTe(6ML)/ZnSe(8ML) SLs with 20 periods and different interface termination (Be-Se interface and Zn-Te interface). Fig. 4 shows valence band spectra near threshold for the two heterostructures with different interface terminations with spectra of the bulk reference samples. The spectra for the SL with a ZnTe interface and the BeTe bulk sample are very similar. In this heterostructure the Be atoms should be surrounded only by Te atoms, which indeed seems to be the case. However, the difference between BeSe interface and BeTe sample is obvious. In this heterostructure there should be a ratio of BeTe to BeSe layers of 5:1. Thus, a spectrum dominated by the BeTe lineshape would be expected. The comparison of the spectra of the SL with BeSe interface and the BeSe bulk sample indicates a strong intermixing at the BeSe interfaces. In contrast, the ZnTe interface seems to be more abrupt, as it resembles the BeTe reference spectrum much more closely.

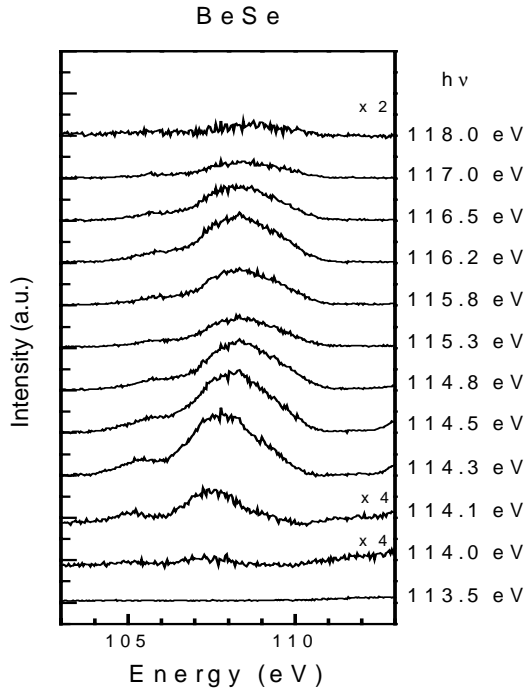


Fig. 3 Excitation-energy dependent XE-spectra of BeSe(100). The transitions for lowest excitation energy (114.1 eV) occurs at the X-point. The transitions with the highest emission energy (116.2 eV) correspond predominantly to the Γ -point.

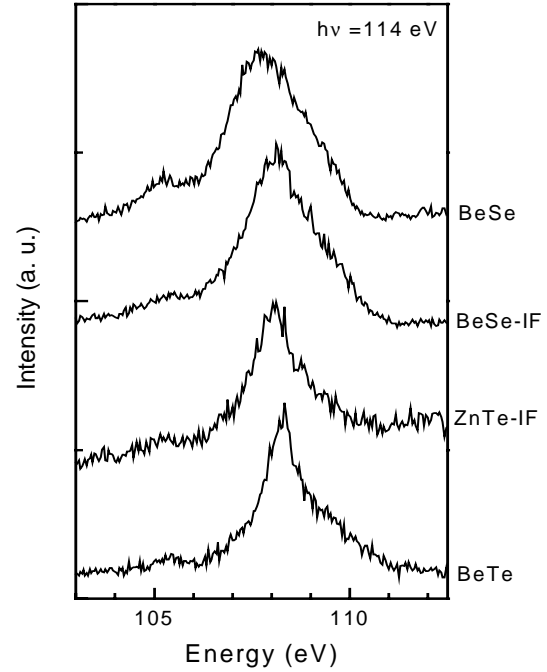


Fig. 4 Valence band spectra near threshold for two SLs with different interface termination. The spectrum of the ZnTe-interface superlattice is similar to the BeTe reference sample. This indicates an abrupt interface. For the BeSe interface also spectrum with a BeTe-lineshape like is expected. The comparison with the BeSe reference sample shows a strong intermixing.

CONCLUSION

The experimental results confirm that XES can be used as a bulk-sensitive method to study the electronic bulk band structure of solids in detail. Moreover, using XES spectra as (bulk) reference allows a “fingerprint-approach” to the electronic and chemical structure of buried superlattices and thin interfaces. In the present experiment this approach could be utilized to investigate the atomic intermixing of BeTe/ZnSe-superlattices, and it could be derived that superlattices with BeSe interface show strong intermixing, while ZnTe-terminated interfaces are identified to be more abrupt.

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Principal investigator: Prof. Dr. Eberhard Umbach, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany. E-mail: umbach@physik.uni-wuerzburg.de. Telephone: ++49-931-888-5755.